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PROGRAM LIBRARY

DECUS NO.	8-323
TITLE	CRC (Convert Peak Heights On An Auto-Analyzer Chart to PPM and Percentage)
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SOURCE LANGUAGE	FORTRAN D

CRC (Convert Peak Heights On An Auto-Analyzer Chart To PPM And Percentage)

DECUS Program Library Write-up

DECUS No. 8-323

ABSTRACT

CRC is a program to convert peak heights on an Auto-Analyzer chart to ppm and percentage. The program:

1. Converts the standard peak heights (known ppm concentration) read from an Auto-Analyzer chart to optical density.
2. Computes the linear regression $y = a + bx$.
3. Converts the sample peak heights (unknown ppm concentration) to optical density and ppm.
4. Subtracts the blank values, if any, from the samples.
5. Calculates percentage concentration.

Any number of standards may be used and any number of sets of standards and samples may follow.

TAPES REQUIRED

1. Form of program tape - The program is written in the PDP-8 FORTRAN-D language and is in the source language.
2. Form of data tape - The data to be analyzed should be punched onto paper tape in the ASCII code. The data should start with the total width of the chart. For each set of standards there should be:
 1. Number of standards.
 2. Peak height (x) and concentration (y ppm) for each standard.
 3. Peak heights (x) of blank solutions.
 4. For each sample
 - a) number of the sample
 - b) weight of sample taken for digestion (g)
 - c) final solution volume (ml)
 - d) dilution of solution used for the Auto-Analyzer
 - e) sample peak height (x)

e.g.

Number of standards	4	
Width of the chart (cm)	27.95	
Standards (x then y)	2.20	0.0
	11.70	0.5
	15.90	1.0
	18.20	2.0

Peak height of Blank Solutions (x)	2.45	2.50
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For each sample	a	b	c	d	e
1.	0.4	50	5	12.50	
2.	0.4	50	5	14.60	

Where a further set of standards is required punch a negative sign before the number of the last sample then the number of the next set of standards. On the last sample of all punch zero instead of the sample number; this will stop the program.

OPERATING INSTRUCTIONS

.FORT

*OUT-S:CRC

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*IN-R:

Program tape in high-speed reader

* ↑

*READY

↑

Data tape in high-speed reader

Switch on high-speed punch.

OUTPUT

For each sample peak the program prints the number of the sample, ppm and percentage. Output is by high-speed punch.

METHOD

This program is only applicable when:

1. The zero aperture on the recorder has been to 0° Transmission.
2. No range expansion has been used on the recorder.
3. There is no drift in the reagent baseline.

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C

;CHART READER PROGRAM

READ 2,106,WOC

106;FORMAT (E)

C

;CONVERT TO OP.DEN. AND DO REGRESSION.

WRITE 2,105

105;FORMAT (/," PPM %",/)

3;READ 2,100,N

100;FORMAT(I)

SUMX=0.0

SUMY=0.0

SUX2=0.0

SUY2=0.0

SUXY=0.0

Z=N

DO 6 NI=1,N

READ 2,101,X,Y

101;FORMAT (E,E)

DEN=0.0

DEN=WOC-X

X=WOC/DEN

X=LOGF(X)*0.4343

SUMX=SUMX+X

SUMY=SUMY+Y

SUX2=SUX2+X**2

SUY2=SUY2+Y**2

SUXY=SUXY+X*Y

6;CONTINUE

SXXY=SUMX*SUMY

XBAR=SUMX/Z

YBAR=SUMY/Z

SXX2=SUX2-(SUMX*SUMX/Z)

SXYB=SUXY-(SXXY/Z)

RGCF=SXYB/SXX2

RGCT=YBAR-(RGCF*XBAR)

C

;CONVERT CHART READING FOR BLANK TO OP.DEN.

READ 2,102,BL1,BL2

102;FORMAT(E)

DEN=0.0

DEN=WOC-BL1

BL1=(WOC/DEN)

BL1=LOGF(BL1)*0.4343

DEN=0.0

DEN=WOC-BL2

BL2=WOC/DEN

BL2=LOGF(BL2)*0.4343

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C      ;DO PREDICTION FOR BLANKS
      BBX1=BL1*RGCF
      BCO1=BBX1+RGCT
      BBX2=BL2*RGCF
      BCO2=BBX2+RGCT
      BL=(BCO1+BCO2)/2.0
C      ;CONVERT CHART READING FOR SAMPLE TO OP.DEN.
      1;READ 2,103,NO,WT,VOL,DIL,SAMP
      103;FORMAT(I,E,E,E,E)
      DEN=0.0
      DEN=WOC-SAMP
      SAMP=(WOC/DEN)
      SAMP=LOGF(SAMP)*0.4343
C      ;DO PREDICTIONS FOR SAMPLES.
      SBX=SAMP*RGCF
      CONC=SBX+RGCT
      IF(BL)5,4,4
      4; CONC=CONC-BL
      5; SAMP=CONC*(VOL*DIL)/(10000.0*WT)
      WRITE 2,104,NO,CONC,SAMP
      104;FORMAT(I,E,E,/)
      IF(NO)3,2,1
      2;STOP
      END

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